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13. ABSTRACT

The investigator was able to give a complete mathematical analysis for a self-consistent dynamic model for rf sheaths in the frequency range between the ion and electron plasma frequencies for arbitrary collision parameters and arbitrary rf sheath voltages.

Based on the above analysis, the investigator developed an algorithm which permits a complete numerical solution of the problem in its full generality without any restrictive assumptions.

Using the developed algorithm, the investigator has computed the sheath characteristics for Argon and Helium.

The computed results were compared with those found in known rf sheath theories and with those obtained experimentally at GTE Laboratories for a wide range of discharge conditions. It was found that our mathematical model matches the experiment better than any of the existing models. It is most complete and generalized model for the rf sheath in capacitive re discharges.

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TECHNICAL REPORT
for the period June 1, 1991–September 30, 1994
AFOSR–91–0233
Mathematical Modeling in Plasma Physics

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The proposed project consisted of three parts:

I. To study the transition from the constant ion mobility regime at the center of the plasma to the space–charge regime at the plasma boundary in the static bounded plasma problem.

II. To understand and describe both analytically and numerically the characteristics for the dynamic nonlinear large amplitude perturbation model of the plasma sheath that has been developed by V. Godyak as the basis of the theory of radio frequency discharges.

III. To find a mathematical model for determining the small signal capacitance of the plasma sheath at intermediate frequencies.

A number of problems for a dynamic model of the sheath have been successfully addressed by the PI in collaboration with V. Godyak [1,2]. The intent of Part II of the proposal was to modify the model and the algorithm in [1,2] so it becomes applicable for Argon, and to compare the numerical and experimental data, in order to check the model and the theory further. During the period covered in this report, the goals of this part of the project have been achieved:

1. The investigator was able to give a complete mathematical analysis for a self–consistent dynamic model for rf sheaths in the frequency range between the ion and electron plasma frequencies for arbitrary collision parameters and arbitrary rf sheath voltages.

2. Based on the above analysis, the investigator developed an algorithm which permits a complete numerical solution of the problem in its full generality without any restrictive assumptions.

3. Using the developed algorithm, the investigator has computed the sheath characteristics for Argon and Helium.

4. The computed results were compared with those found in known rf sheath theories [4-8], and with those obtained experimentally at GTE Laboratories for a wide range of discharge conditions. It was found that our mathematical model matches the experiment better than any of the existing models. It is the most complete and generalized model for

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the rf sheath in capacitive rf discharges.

Based on the obtained results, two papers have been written by the PI:

"A comparison of rf electrode sheath models" (with V. Godyak and R. Piejak), IEEE Trans. of Plasma Sci., 21, 4, 1993

"Solving the mathematical model of the electrode sheath in symmetrically driven rf discharges" (with V. Godyak), J. Comp. Phys., 111, 2, 347–353, 1994.

In the first paper analytical expressions for the electrode sheath width were obtained for different time-averaged and dynamic models of capacitive rf discharges. It has been found that in all models under consideration, the sheath widths practically coincide if they are expressed in terms of the dc sheath voltage and the electrode ion current to the rf electrode.

In the second paper, a complete mathematical analysis was given for a self-consistent dynamic model of rf sheaths in the frequency range between the plasma ion and electron frequency. Arbitrary collision parameters and arbitrary rf sheath voltages have been considered. Based on this analysis an algorithm has been developed to solve numerically the mathematical problem in its full generality. The developed method was then used to obtain the electrode sheath characteristics and to study their dependence on the rf sheath conductivity parameter for Argon.

In somewhat more detail, the results obtained to date can be summarized as follows.

A self-consistent hydrodynamic model for the sheaths of a symmetrically driven rf discharge was formulated in Ref. [3]. In Ref. [1], this model was generalized. In the model, under the action of the rf field, the plasma–sheath interface exhibits an oscillatory behavior. Therefore, the position of the plasma–sheath interface at any given time θ can be described by a periodic function $\lambda(\theta)$ that achieves its maximum λ_1 at some time $\theta = \theta_1$ and its minimum λ_2 at $\theta = \theta_2$. To the right of the moving interface, in the plasma, the electron density is equal to the ion density (plasma neutrality). To the left of the moving interface, in the sheath, the electron density is equal to zero (space charge). From the physical point of view the generalized model [1] is the most accurate and justified, mathematically, however, it leads to a complicated moving boundary problem that in the past has had to be simplified in order to be solved. A number of such simplified models appeared in the literature (see [4-8]), but the mathematical simplification have lead to physical inconsistencies and inaccuracies. In Ref. [1], we worked out the generalized model under the single restrictive assumption that the function λ is symmetric with respect to its minimum position λ_2. A comparison of the analytical and numerical solutions of the mathematical model with the available experimental results for mercury vapor have demonstrated a good agreement in corresponding values. The mathematical analysis, which underlies the numerical results, can be found in [2]. In general, however, λ is not symmetric with respect to its minimum position λ_2, and always imposing such an assumption might lead to inaccuracies for other gases. Indeed, such an assumption leads to corresponding symmetries in the solutions to the problem. Such symmetry, however, is

not to be expected. In fact, asymmetry becomes more pronounced for large oscillations of the plasma–sheath interface. How to solve the moving boundary problem, which describes the generalized model [1], without any restrictive assumptions or simplification has up until now remained an open question. We were able to answer this question by giving a detailed mathematical analysis of the generalized model. This enabled us to solve the problem numerically in its full generality, and to obtain the characteristics of the electrode sheath. Using the numerical results, we were also able to obtain an approximation formula for the sheath characteristics for arbitrary sheath voltages and collision parameters. This formula is similar to the Child–Langmuir Law and can easily be used for the experimental modeling of rf discharges.

In most applications, one has to deal with bounded plasmas. Our approach can be used for any bounded plasma created by rf antennas or rf electrodes.

The above results led to the following new problem that originally has not been proposed. In order to solve the model for the sheath, one has to specify the boundary condition at the plasma-sheath interface which would provide a smooth transition from the plasma to the sheath. Since there is no strict boundary between the plasma and the sheath, it is not obvious how to determine such a boundary condition. Most frequently the electric field at the plasma-sheath boundary E_1 is chosen to be zero. This choice results in discontinuities of the gradients of the potential, plasma-density, and velocity, and in some cases it leads to an infinite sheath width. Several attempts have been made to remove these discontinuities by introducing transition layers. Another way to chose the boundary condition at the plasma-sheath interface is to specify the value of the electric field where the plasma neutrality is violated by setting $E_1 = T_e/\lambda_{D_1}$, where T_e is the electron temperature and λ_{D_1} is the electron Debye radius at the plasma-sheath boundary. This nonzero boundary condition for the electric field has been introduced by Godyak [9], and has previously been used by the PI to solve the static sheath model and the dynamic sheath model. However, the precise value for the electric field at the plasma-sheath interface is still being disputed. This dispute leads to the question about the effects of choice of boundary conditions on the sheath characteristics. This question has been addressed by the PI in the paper

"Effects of boundary conditions in the dynamic model of the rf sheath" (with V. Godyak), IEEE Trans. Magnetics, 30, 5, 1994.

Some of the results in this paper were presented at the Conference on the Computations of Electromagnetic Fields (COMPUMAG) in Miami on November 5-6, 1993, and appeared in the COMPUMAG Conference Records, 1993.

In that paper, the calculations were performed for the benchmark modeling case of the symmetrically driven rf discharge in Argon at different values A of the normalized electric field at the plasma–sheath interface: $A = 0$; -0.1; -0.3; -0.5; -0.7; -0.9; -1. The results that have been obtained show that even for relatively high rf sheath voltages, both the dc sheath voltage and the rf sheath capacitance depend in a significant way on the choice of the value for the electric field at the plasma–sheath interface. These results are surprising since for high rf sheath voltages, it has always been believed that the sheath

the sheath characteristics behave asymptotically and are not sensitive to the choice of the boundary conditions. Thus, the question about the choice of boundary condition at the plasma–sheath interface for an adequate rd sheath model is indeed important and relevant. An analysis given by Riemann in [10] suggests that $|A| \approx (\lambda_D/L)$, where L is the plasma width. For rf discharges encountered in applications, this value is much smaller than 1. On the other hands, Godyak's boundary condition suggests that $A = -1$. It remained to be investigated which values of A are appropriate. Such an investigation has been conducted by the PI for the static bounded plasma problem (see Part I). The obtained results will be described below.

During the period covered by this report, the PI has also been working on the static bounded plasma problem with finite nonneutrality. A number of problems concerning the static bounded plasma problem have been addressed by the PI in collaboration with Godyak in [11]. In that paper, the hydrodynamic models for the plasma and the sheath have been studied separately using Godyak's boundary condition. In the plasma model, one assumes that the ion density equals the electron density (quasineutrality). In actual applications, this assumption can be made with sufficiently high accuracy in the center of the plasma. Closer to the boundary this is no longer true. In the sheath model, one assumes that the electron density equals zero. This assumption can be justified only very close to the wall. These facts immediately raise an important questions. In what region can the solution of the total bounded plasma problem be approximated by the solutions of the plasma and the sheath models? In order to answer this question, a mathematical analysis of the static model has been given, and all the needed algorithms have been developed. The following results for the collisionless case with the nonneutrality parameter $q = 0.01$ have been obtained:

1. Using an iteration method we have found the position of the wall: $x_w = 0.6558$.

2. The plasma model approximates the bounded plasma problem in the region $x \leq 0.56$.

3. The sheath model approximates the bounded plasma problem in the region $0.63 \leq x \leq x_w$.

4. In the region $0.56 < x < 0.63$, the bounded plasma problem cannot be approximated by either the plasma or the sheath model. This region corresponds to the presheath region.

These results lead to the following important question. What position of the plasma–sheath interface is specified by Godyak's boundary condition, and what position is specified by Riemann's boundary condition? In order to study this problem, we have solved the plasma and the sheath models varying the boundary condition at the plasma–sheath interface. Comparing the so obtained solutions with the solution of the bounded plasma problem the following has been found:

5. Godyak's boundary condition specifies the position at the plasma–sheath interface at $x = 0.63$. Therefore, this boundary condition can indeed be used as an initial con-

dition for the sheath model to approximate the bounded plasma problem in the region $0.63 \leq x \leq x_w$.

6. Riemann's boundary condition specifies the position at the plasma–sheath interface at $x = 0.56$. This boundary condition can be used as a boundary condition for the plasma model to approximate the bounded plasma problem in the region $0 \leq x \leq 0.56$.

It becomes obvious from the above results that one cannot just combine the solutions of the plasma and the sheath models to obtain an accurate approximation of the solution of the bounded plasma problem. In order to find an accurate approximation of the bounded plasma problem one would have to model not only the plasma and the sheath, but also the presheath. This conclusion lead to another question. How relevant is the presheath in applications? In order to answer this question, we have computed the low frequency capacitance using the total plasma model, and using the sheath model. A comparison of the obtained results has shown the following:

7. In some applications the presheath can be ignored and the bounded plasma problem can indeed be modeled by the plasma and the sheath models separately. The so obtained integral characteristics of the problem are within the accuracy of the experiment.

The preliminary findings concerning the static bounded plasma problem were presented at the IEEE International Conference on Plasma Science, Santa Fe, New Mexico, June, 1994. A detailed description of the above results is currently being prepared for publication.

During the period covered by this report, the following papers have been published by the PI:

1. Rf sheath parameters for Argon and Helium discharges, Conference Records, IEEE International Conference on Plasma Science, Williamsburg, VA, June, 1991 (with V. Godyak and R. Piejak).

2. Sheath capacitance at low and high frequencies (with V. Godyak), Proceed. XX Int. Conf. on Phenomena in Ionized Gases, Pisa, Italy, July, 1991.

3. A Hartman–Grobman Theorem for maps, Proceed. Int. Conf. on Theory and Appl. of Diff. Eq., Edinburg, Texas, May, 1991, in "Ordinary and delay differential equations", Eds. J. Hale and J. Wiener, Pitman Research Notes in Mathematics Series, 1992.

4. A moving boundary value problem in Plasma Physics (with V. Godyak), Proceed. III Potsdam–V Kiev Int. Workshop on Nonlinear Processes in Physics, Potsdam, NY, August, 1991, in "Nonlinear Processes in Physics", Eds. A.S. Fokas, D.J. Kaup, A.C. Newell, V.E. Zakharov, Springer-Verlag, 1993.

5. A Hartman–Grobman Theorem for a class of retarded functional differential equations, J. Math. Analysis and Appl., 175, 1993.

6. A comparison of rf electrode sheath models (with V. Godyak and R. Piejak), IEEE Trans. of Plasma Sci., 21, 4, 1993.

7. Solving the mathematical model of the electrode sheath in symmetrically driven rf discharges (with V.A. Godyak), J. Comp. Phys., 111, 2, 347–353, 1994.

8. Effects of boundary conditions in the dynamic model of the rf sheath, (with V.A. Godyak), IEEE Trans. Magnetics, 30, 5, 3100–3103, 1994.

During the period covered by this report, the following presentations at international conferences have been given by the PI:

1. Rf sheath parameters for Argon and Helium discharges, IEEE International Conference on Plasma Science, Williamsburg, VA, June, 1991.

2. Sheath capacitance at low and high frequencies (with V. Godyak), Proceed. XX Int. Conf. on Phenomena in Ionized Gases, Pisa, Italy, July, 1991.

3. Mathematical modeling in Plasma Physics, invited participant, III Potsdam–V Kiev International Workshop on Nonlinear Processes in Physics, Clarkson University, Potsdam, New York, August, 1991.

4. A Hartman–Grobman theorem for maps, SIAM Conference on Applications of Dynamical Systems, Snowbird, Utah, October, 1992.

5. Effects of boundary conditions in the dynamic model of the rf sheath, COMPUMAG 9th Conference on the Computation of Electromagnetic Fields, Miami, Florida, November, 1993.

6. Approximation of the bounded plasma model by the plasma and the sheath models, IEEE Int. Conf. on Plasma Science, Santa Fe, New Mexico, June, 1994.

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